Adiabatic quantum computation: Enthusiast and Sceptic's perspectives

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Enthusiast's perspective: We analyze the effectiveness of AQC for a small rank problem Hamiltonian H_F with the *arbitrary* initial Hamiltonian H_I. We prove that for the generic H_I the running time cannot be smaller than $O(\sqrt{N})$, where N is a dimension of the Hilbert space. We also construct an explicit H_I for which the running time is indeed $O(\sqrt{N})$. Our algorithm can be used to solve the unstructured search problem with the *unknown* number of marked items.

Sceptic's perspective: We show that for a *robust* device, the running time for such H_F cannot be much smaller than $O(N/\ln N)$.

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Overture.—Adiabatic quantum computation (AQC) (*e.g.* [1]) is a Hamiltonian-based model of quantum computation. The idea behind AQC is that finding the ground state of a problem Hamiltonian H_F solves interesting computational problems. In the abstract setting, let H_I, H_F be a pair of hermitian $N \times N$ matrices, with $N \gg 1$. Consider the interpolating Hamiltonian $H(s)$ of the form

$$H(s) := (1 - f(s))H_I + f(s)H_F\,, \tag{1}$$

where f is a monotone function on $[0,1]$ satisfying $f(0) = 0$, $f(1) = 1$. We will denote by P_I (respectively P_F) the spectral projection on the ground state energy E_I (E_F) of the matrix H_I (H_F). We prepare the initial state of the system $\psi(0)$ in the (*a-priori* known) ground state $\psi_I \in Range\, P_I$ of the Hamiltonian H_I [2], and let the system evolve according to the (scaled) Schrödinger equation:

$$i\dot{\psi}_\tau(s) \;=\; \tau H(s)\psi_\tau(s)\,, \quad \psi_\tau(0) \;=\; \psi_I\,. \tag{2}$$

The adiabatic theorem of quantum mechanics ensures that under certain conditions the evolution $\psi_\tau(1)$ of the initial state stays close to the $Range\, P_F$. For AQC to be a potent quantum algorithm, the running (*i.e.* physical) time τ in Eq. (2) must be much smaller than N. Although AQC attracted a considerable interest in physics and computer science communities, the quantitative characterization of the speed up in its use remains at large unknown. The core issue here is related to the extreme sensitivity of the adiabatic behavior to the spectral structure of the operator $H(s)$. Specifically, the deviations *may* become large when the gap $g(s)$ between the ground state of $H(s)$ and the rest of its spectrum is small in the vicinity of some instant $s \in [0,1]$.

The traditional approach to the problem so far was to estimate this minimal gap [3]. Putting a few rare exceptions aside (*e.g.* [4]), it is usually a very hard task. This explains why, generally speaking, not much light was shed on the effectiveness of AQC. Let us note that the estimates of the running time involving the gap $g(s)$ alone provide only the upper bound on the optimal running time τ. In reality τ can be much smaller.

In this paper, we discuss the reliable upper and lower bounds on the optimal value of τ, circumventing the estimates on the size of the gap. Our method is applicable for a particular class of problem Hamiltonians, satisfying the following hypothesis.

Assumption 1. *The problem Hamiltonian is of the small rank: $Rank(H_F) := m \ll N$.*

Even in this narrower context, there is no unequivocal riposte to whether AQC is indeed efficient, as we shall see. As often happens in theoretical deliberations, the answer depends, to some extent, on the degree of your zeal. To keep the discussion balanced, we present two different perspectives: The first one is on the optimistic side while the second one is rather pessimistic in its nature. To this end we set a stage for two close acquaintances, Messrs. Enthusiast and Sceptic, and let the wise Reader judge who of them is closer to the mark.

Let us note that for AQC to work, it suffices to ensure that $\psi_\tau(1)$ has a non trivial overlap with the range of H_F, which we will encode in the requirement $\|P_F\psi_\tau(1)\| \geq 1/5$, [5]. Another issue that usually arouses certain degree of confusion, which we want to avoid, is a normalization of $H(s)$. To that end, we will use the calibration $\|H_I\| = \|H_F\| = 1$. One should bear this convention in mind when performing comparison with other results.

The rest of the paper is organized as follows: We first present the discussion from Enthusiast and Sceptic's points of view, indicating briefly the intuition behind the corresponding assertions. We then give proofs of Theorems 3 and 4 (the rest of the proofs can be found in [6]). Now we pass the baton to Mr. Enthusiast.

Enthusiast's perspective.—To formulate the result, let me introduce a set of the related parameters. First, I want to quantify the overlap between the initial state ψ_I and the problem Hamiltonian. Namely, let $\delta_1 = \|H_F\psi_I\|$, let $\delta_2 = \|P_F\psi_I\|$, and let $\delta_3 = \|Q_F\psi_I\|$, where Q_F is a projection onto $Range\, H_F$. Note that for a generic H_I all δ's are small, with δ_1 and δ_3 being $O(\sqrt{m/N})$, while

$\delta_2 = O(\sqrt{m'/N})$. Here m' is a dimension of *Range* P_F. Second, I want to distinguish between E_F and the rest of the spectrum of H_F, which I will assume henceforth are separated by the gap g_F. Finally, since I don't want to assume that H_F is sign definite and given that $\|H_F\| = 1$ by convention, the energy E_F will show up in the estimates. The prototypical example covered by our results is the generalized unstructured search (GUS) problem, which can be cast in the following form: Suppose H_F is diagonal with the *unknown* number of entries equal to -1 and the rest of the entries equal to zero (so that $H_F = \mathbf{1} - P_F$). Pick $H_I = -|\psi_I\rangle\langle\psi_I|$ with $\psi_I = N^{-1/2}(1, \ldots, 1)$. Then the corresponding parameters are $\delta_3 = \delta_2 = \sqrt{m/N}$, $E_F = -1$, and $g_F = 1$.

The pair of results below, coupled together, gives fairly tight lower and respectively upper bounds on the optimal running time in AQC.

Theorem 1. *Consider the interpolating family Eq.* (1) *with an arbitrary* f. *Then the running time* τ_- *in Eq.* (2) *for which* $\|Q_F \psi_{\tau_-}(1)\| \geq 1/5$ *satisfies*

$$\tau_- \;\geq\; \frac{1 - 5\delta_2}{5\delta_1}\,, \qquad \textit{for} \quad \delta_2 < 1/5\,. \tag{3}$$

The quantitative measure of how much $\psi_\tau(s)$ deviates from ψ_I is encoded in the size of the commutator $[P_I, H(s)]$. Hence one expects to see the deviation from ψ_I over the time τ such that $\tau \cdot \|[P_I, H(s)]\| = O(1)$. Since P_I commutes with H_I while $\|[P_I, H_F]\| \leq 2\delta_1$, we get $\|[P_I, H(s)]\| \leq 2\delta_1$ for all s and the bound in Eq. (3) follows up to a constant.

Let me note that the similar, albeit less sharp (with the wrong dependence on m) lower bound was recently established in [7].

Theorem 2. *Suppose* $\delta_3/g_F = O(1/\ln N)$, *Then there exists an explicit rank one* H_I *and an explicit function* f *such that* $\|P_F \psi_{\tau_+}(1)\| \;\geq\; 1/5$ *for*

$$\tau_+ \;=\; \frac{C(1 - E_F)}{|E_F|\,\delta_2}\,, \tag{4}$$

for any $C \in [1/3, 2/3]$.

For $N \gg m$ the requirement on δ_3/g_F is typically satisfied. Note also that $\tau_-/\tau_+ \approx \sqrt{m'/m}$. This is not particularly surprising, as in Theorem 1 the aim was to ensure that $\psi_{\tau_-}(1)$ has an overlap with the range of H_F, whereas in Theorem 2 we want $\psi_{\tau_+}(1)$ to overlap with *Range* P_F.

The choices in the theorem are: $H_I = -|\psi_I\rangle\langle\psi_I|$ and a (non adiabatic) parametrization $f(s)$ is given by

$$f(s) \;=\; \begin{cases} 0\,, & s = 0 \\ \alpha \equiv \frac{1}{1 - E_F}\,, & s \in (0,1) \\ 1\,, & s = 1 \end{cases}\,.$$

That means we move diabatically (instantly) to the given point of the path, stay there for the time τ_+, and then move quickly again to the end of the path. Such f is in fact optimal for the Grover's problem.

The intuition behind this assertion is as follows: With the above choice for $f(s)$

$$\psi_\tau(1) \;=\; e^{-i\alpha\tau_+ \cdot (E_F P_I + H_F)} \psi_I.$$

Note now that the ground state energy of $E_F P_I$ matches that of H_F and differs from the energies of its excited states. Let X be a subspace spanned by vectors in the ranges of P_I and P_F, and let $X^\perp$ be its orthogonal complement (so that $X \bigoplus X^\perp$ is the whole Hilbert space). As usual in adiabatic setting, the transitions between X and $X^\perp$ are suppressed due to fast oscillations caused by the energy differential. Therefore the initial state ψ_I slowly precesses in the X subspace, and by choosing the right value for τ_+ one can find the evolved state sufficiently close to *Range* P_F. The argument identical to the one in Theorem 1 shows that the running time τ_+ is roughly

$$\frac{1 - E_F}{|E_F|} \cdot \frac{1}{\|[P_I, P_F]\|} = \frac{1 - E_F}{|E_F|} \cdot \frac{1}{2\delta_2}\,.$$

Since the precession is very slow, τ_+ is fairly robust.

This assertion can be seen as an extension of the classical result of Farhi–Gutmann [8] on the Grover's search problem. For GUS the parallel result was established for the quantum circuit model (QCM) in [9].

Theorem 2 uses values of E_F and $\delta_2 = \|P_F \psi_I\| = O(1/\sqrt{N})$ as the input. In many important applications (such as GUS) the value of δ_2 is unknown. To this end, we prove the following assertion.

Theorem 3. *Suppose that the value of* E_F *is known. Then there is a Hamiltonian – based algorithm that determines* δ_2 *with* $1/N^2$ *accuracy and requires* $O((\ln N)^2)$ *of the running time.*

Note that the combined running time in Theorems 2 and 3 remains $O(\sqrt{N})$. The algorithm used in the proof is inspired by the mean ergodic theorem and makes use of the fact that the survival probability $c_F(t) = \langle\psi_I | e^{itH_F} \psi_I\rangle$ is directly measurable in AQC framework. For GUS this problem is known as quantum counting and was analyzed in QCM framework in [9].

Enthusiast's summary.—Theorem 1 tells us that for a generic H_I the running time cannot be smaller than $O(\sqrt{N})$. Theorems 2 and 3 construct the explicit H_I and the parametrization $f(s)$ so that $\tau = O(\sqrt{N})$. I have assumed that the ground state energy E_F of H_F is known with the $1/N$ accuracy.

Sceptic's perspective.—Let me first point out two shortcomings of the method which is usually employed in estimation of the running time of AQC (*e.g.* [4] for the Grover's problem and [10]). The technique hinges on a choice of a parametrization f such that $\dot{f}(s)$ is small

whenever the instantaneous spectral gap $g(s)$ is small [11]. To construct such f, one need to know the values s_j for which $g(s_j) = O(N^{-1/2})$ with high precision. Such analysis requires the detailed information about the spectral structure of H_F. The similar issue is present (albeit to a lesser extent) in the Enthusiast's approach, as one still needs to know E_F. Even if this technical hurdle can be overcome, the extreme susceptibility of $\psi_\tau(1)$ to the parametrization f poses a radical problem in practical implementation. Indeed, it is presumably extremely difficult to enforce $\dot f = 0$ for a long stretch of the physical time, as the realistic computing device inevitably fluctuates. So in the robust setting one can assume that for any given moment s_0 the value $\dot f(s_0)$ is greater than some small but fixed κ. We can then as well consider the functions f in the robust setting that satisfy $\dot f(s) > \kappa$ for *all* values of s.

To understand how the robust system evolves, let me consider the following semi-empiric argument, substantiated in Theorem 4 below. One can show [6] that for a finite rank matrix H_F the minimum value g of the gap $g(s)$ between the ground state energy $E(s)$ of $H(s)$ and the rest of the spectrum of $H(s)$ is $O(\delta_3)$. Let $g = g(s_0)$, then one can introduce two different time scales: τ_1 and τ_2. We set $\tau_1 = \Delta^{-1}$, where Δ is a gap between the two smallest eigenvalues of $H(s_0)$ and the rest of its spectrum. The scale τ_2 is associated with a two level system corresponding to the restriction of the Hilbert space to the spectral subspace of these two eigenvalues. Typically, $\tau_1 \ll \tau_2$, and ψ_τ stays close to the ground state provided $\tau \gg \tau_2$. If $\tau_1 \ll \tau \ll \tau_2$, then ψ_τ will still stay close to the range of the above spectral subspace. However, it will behave as if the avoided level crossing is a true level crossing, with evolution following the first excited state rather than the ground state (see Figure 1). To estimate τ_2 let me consider a two level system of the form

$$K(s) \;=\; \begin{bmatrix} 1-f(s) & \delta f(s) \\ \delta f(s) & f(s) \end{bmatrix} . \qquad (5)$$

Assuming that f is differentiable, the Landau–Zener formula shows that for $K(s)$ the corresponding time scale is $\tau_2 \approx \dot f(s_0)\,\delta^{-2}$. The value of the minimal gap here is equal to $\delta\sqrt{1+\delta^2} \approx \delta$. Since for $H(s)$ the value of g is roughly δ_3, we see that ψ_τ stays close to the ground state of $H(s)$ only if

$$\tau \;>\; \dot f(s_0)\cdot(\delta_3)^{-2} \;=\; \dot f(s_0)\cdot O(N)\,.$$

Hence in the robust setting, where $\dot f$ cannot be too small at any given instant, there is no significant speed up in using AQC. The result below reaffirms this argument for the case of the initial Hamiltonian H_I of the small rank. In what follows, Q_I will denote the projection onto *Range* H_I, with $\delta := \|Q_I Q_F\|$.

Theorem 4 (Robust lower bound on the running time)**.** *Suppose that f in Eq. (1) is differentiable and satisfies $\dot f(s) \ge \kappa > 0$ for $s \in [0,1]$. Then, if $\tau < \tau_r = O\left(\frac{-\kappa}{m^2\delta^2 \ln \delta}\right)$, we have*

$$|\langle\psi_I|\psi_\tau\rangle| \;>\; \frac{2\sqrt{6}}{5} + \delta\,. \qquad (6)$$

Hence the running time τ for which $\|Q_F\psi_\tau(1)\| \ge 1/5$ cannot be smaller than τ_r.

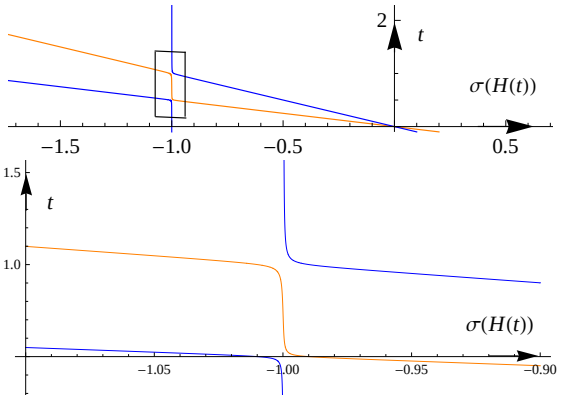

FIG. 1: Illustration for Theorem 4, $N = 10^4$. Top: A pair of relevant eigenvalues of $H(t) := H_I + 2tH_F$ as a function of t, for $H_F = -|e_1\rangle\langle e_1| - \frac{1}{2}|e_2\rangle\langle e_2|$ and $H_I = |\phi_1\rangle\langle\phi_1| - |\phi_2\rangle\langle\phi_2|$. Here $e_1 = (1, 0 \ldots, 0)$, $e_2 = (0, 1, 0, \ldots, 0)$, $\phi_1 = 1/\sqrt{N}(1, \cdots, 1)$, and $\phi_2 = 1/\sqrt{N}(1, \ldots, 1, -1, \ldots, -1)$, with exactly half of -1 so that $\langle\phi_1|\phi_2\rangle = 0$. Bottom: The magnified region of the avoided crossings in the upper panel.

Sceptic's summary.—Theorem 4 tells us that for a generic H_I of the small rank the robust running time τ_r cannot be smaller than $O(N/\ln N)$. Hence AQC is not really effective for the problem Hamiltonians that satisfy Assumption 1.

Proof of Theorem 3. The starting point is a pair of identities, [12]:

$$\begin{aligned} e^{-p}\sum_{k=1}^{\infty}\frac{p^k\sin(k\omega)}{k!} &= e^{p(\cos\omega-1)}\sin(p\sin\omega) \\ e^{-p}\sum_{k=1}^{\infty}\frac{p^k\cos(k\omega)}{k!} &= e^{p(\cos\omega-1)}\cos(p\sin\omega)\,. \end{aligned} \qquad (7)$$

In particular, if $1-\cos\omega > \Delta$, each term in Eq. (7) is bounded by $e^{-p\Delta}$ and therefore is smaller than $1/N^2$ provided $p = 2\ln N/\Delta$. On the other hand, the remainders to the partial sums (up to $k = L$) in Eq. (7) are $O(p^L/L!)$ provided the latter quantity is small. Combining these observations, we get

$$e^{-p}\sum_{k=1}^{p}\frac{p^k e^{ik\omega}}{k!} = \begin{cases} 1+O(1/N^2)\,, & \omega = 0 \\ O(1/N^2)\,, & 1-\cos\omega > \Delta \end{cases},$$

for $p = 2\ln N/\Delta$ and $\Delta < 1$. Hence

$$e^{-p}\sum_{t=1}^{p}\frac{p^k}{k!}\,\langle\psi_I|e^{it(H_F-E_F)}\psi_I\rangle \;=\; (\delta_2)^2 + O(1/N^2)\,, \quad (8)$$

for $p = 2\ln N/(1-\cos g_F)$. The total running time is $\sum_{t=1}^{p} t = O((\ln N)^2)$. □

Proof of Theorem 4. For a solution $\psi_\tau(s)$ of (2), let

$$\phi_\tau(s) := \; e^{ih(s)\tau\, E_I}\psi_\tau(s)\,,\; h(s) = \int_0^s (1-f(r))\,\mathrm{d}r\,. \quad (9)$$

Then one can readily check that $\phi_\tau(s)$ satisfies IVP

$$i\dot{\phi}_\tau(s) \;=\; \tau\hat{H}(s)\phi_\tau(s)\,,\quad \phi_\tau(0) \;=\; \psi_I\,, \qquad (10)$$

where $\hat{H}(s) = (1-f(s))\,(H_I - E_I) \,+\, f(s)\,H_F$. Clearly $|\langle\psi_I|\psi_\tau\rangle| = |\langle\psi_I|\phi_\tau\rangle|$. Let

$$B(s) = (f(s)H_F - ((1-f(s))E_I + \epsilon i))^{-1}\,,$$

and let $\phi(s) = \psi_I - f(s)H_F B(s)\,\psi_I$, where ϵ is a small parameter to be chosen later. Omitting the s dependence, we have

$$\hat{H}\phi = -f(1-f)H_I H_F B\,\psi_I + i\epsilon f H_F B\,\psi_I\,. \qquad (11)$$

That means that away from the m values of s for which $B(s)$ has zero eigenvalue, $\|\hat{H}\phi\|$ is very small, since $\|H_I H_F \psi_I\| \le \delta^2$. Note now that

$$\langle\phi(1)|\phi_\tau(1)\rangle \;=\; \langle\phi(0)|\phi_\tau(0)\rangle \,+\, \int_0^1 \frac{d}{ds}\langle\phi(s)|\phi_\tau(s)\rangle\,ds\,. \qquad (12)$$

But $\langle\phi(0)|\phi_\tau(0)\rangle = 1$ and

$$\begin{aligned}|\langle\phi(1)|\phi_\tau(1)\rangle| \;&=\; \left|\langle\psi_I|\phi_\tau(1)\rangle \,-\, \langle\psi_I|\frac{H_F}{H_F - \epsilon\, i}|\phi_\tau(1)\rangle\right| \\ &\le\; |\langle\psi_I|\phi_\tau(1)\rangle| \,+\, \|Q_F\psi_I\| \;\le\; |\langle\psi_I|\phi_\tau(1))| \,+\, \delta\,.\end{aligned}$$

Substitution into Eq. (12) gives

$$1 \,-\, |\langle\psi_I|\phi_\tau(1)\rangle| \;\le\; \left|\int_0^1 \frac{d}{ds}\langle\phi(s)|\phi_\tau(s)\rangle\,ds\right| \,+\, \delta\,.$$

Hence Eq. (6) will follow if

$$\left|\int_0^1 \frac{d}{ds}\langle\phi(s)|\phi_\tau(s)\rangle\,ds\right| \;<\; 1 \,-\, \frac{2\sqrt{6}}{5} \,-\, 2\delta\,. \qquad (13)$$

We have

$$\frac{d}{ds}\langle\phi(s)|\phi_\tau(s)\rangle \;=\; \langle\dot{\phi}(s)|\phi_\tau(s)\rangle \,-\, i\tau\langle\phi(s)|\hat{H}(s)|\phi_\tau(s)\rangle\,.$$

We bound the first term on the right hand side by $\|\dot{\phi}\|$ and the second one by $\tau\|\hat{H}\phi_\tau\|$. A straightforward computation (using Eq. (11) for the second term) shows that

$$\|\dot{\phi}\| \;\le\; \frac{\dot{f}\delta}{\Delta_\epsilon} \,+\, \frac{2\dot{f}\delta}{(\Delta_\epsilon)^2}\,;\; \|\hat{H}\phi_\tau\| \;\le\; \frac{\delta^2 + \epsilon\delta}{\Delta_\epsilon}\,,$$

where $\Delta_\epsilon(s) := \mathrm{dist}(f(s)\sigma(H_F)\,,\,(1-f(s))E_I + \epsilon\, i)$. Here $\mathrm{dist}(S,z)$ is an Euclidean distance from the set S to the point z in $\mathbb{C}$, and $\sigma(H)$ stands for the spectrum of H.

As a result, we obtain a bound

$$\left|\dot{\overbrace{\langle\phi|\phi_\tau\rangle}}\right| \;\le\; (\dot{f} + \tau\delta + \tau\epsilon)\frac{\delta}{\Delta_\epsilon} \,+\, 2\frac{\dot{f}\delta}{(\Delta_\epsilon)^2}\,.$$

Integrating both sides over s and using the bounds

$$\begin{aligned}&\int_0^1 \frac{\dot{f}ds}{\Delta_\epsilon(s)} \;\le\; -2m\ln\epsilon\,;\quad \int_0^1 \frac{\dot{f}ds}{(\Delta_\epsilon(s))^2} \;\le\; \frac{2m}{\epsilon}\,; \\ &\int_0^1 \frac{ds}{\Delta_\epsilon(s)} \;\le\; -2m\frac{\ln\epsilon}{\kappa}\,,\end{aligned}$$

we can estimate

$$\begin{aligned}&\left|\int_0^1 \frac{d}{ds}\langle\phi(s)|\phi_\tau(s)\rangle\,ds\right| \\ &\qquad\le\; 2m\delta\left(-\ln\epsilon\left(1 + \frac{\tau\delta}{\kappa} + \frac{\tau\epsilon}{\kappa}\right) + \frac{2}{\epsilon}\right)\,.\end{aligned}$$

Hence the required bound in Eq. (13) follows with the choice $\epsilon = 10^{-3}m\delta$, provided $\tau \le -\frac{C\kappa}{\epsilon^2\ln\epsilon}$ where C is a constant. □

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[1] E. Farhi *et al.*, Science **292**, 472 (2001).

[2] The range of the operator A on a Hilbert space X is a collection of all vectors y such that $y = Ax$ for some $x \in X$. The rank of A is a dimension of *Range* A and coincides with the number of non zero eigenvalues for hermitian A. For example, for $A = |\psi\rangle\langle\psi|$ the range consists of vectors proportional to ψ and *Rank* $A = 1$.

[3] We will relate our results with the prior gap-free bounds on τ (namely [7, 8]) in the next section.

[4] W. van Dam *et al.*, 42nd IEEE Symposium on Foundations of Computer Science 279 (2001).

[5] In fact, it suffices to have an overlap of order $1/p(\ln N)$, where $p(x)$ is a polynomial in x.

[6] Z. Cao and A. Elgart, arXiv:1004.4911v1.

[7] L. M. Inannou and M. Mosca, Int. J. Quant. Inform. **6**, 419 (2008).

[8] E. Farhi and S. Gutmann, Phys. Rev. A **57**, 2403 (1998)

[9] G. Brassard *et al.*, Lecture Notes in Comput. Sci. **1444**, 820 (Springer-Verlag, New York/Berlin (1998)).

[10] A. T. Rezakhani *et al.*, Phys. Rev. Lett. **103**, 080502 (2009).

[11] In fact, the Enthusiast's approach brings this strategy to its extreme by choosing $\dot{f}(s) = 0$ for *all* $s \in (0,1)$. One can show [6] that that for the sign definite H_F the number of avoided crossings is exactly equal to m.

[12] I. S. Gradshteyn and I. M. Ryzhik, formulae (1.449), *Table of integrals, series, and products* (Elsevier/Academic Press, Amsterdam, 2007).